Mott-Hubbard Transition of Bosons in Optical Lattices with Three-body Interactions

Bo-Lun Chen,* Xiao-Bin Huang, and Su-Peng Kou†

Department of Physics, Beijing Normal University, Beijing 100875, China

Yunbo Zhang

Department of Physics and Institute of Theoretical Physics, Shanxi University, Taiyuan 030006, China

In this paper, the quantum phase transition between superfluid state and Mott-insulator state is studied based on an extended Bose-Hubbard model with two- and three-body on-site interactions. By employing the mean-field approximation we find the extension of the insulating 'lobes' and the existence of a fixed point in three dimensional phase space. We investigate the link between experimental parameters and theoretical variables. The possibility to obverse our results through some experimental effects in optically trapped Bose-Einstein Condensates(BEC) is also discussed.

I. INTRODUCTION

Quantum phase transitions in ultracold atoms(BEC) exhibit fascinating phenomena and attract much attention since such a system with controllable interactions between atoms had been realized experimentally by loading the condensate into an optical lattice [1]. The behavior of the BEC in optical lattices can be well described by the Bose-Hubbard model [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12] which predicts a superfluid-insulator transition under certain critical conditions for the interatomic interaction strengths. The rich phenomena as well as sophisticated phase diagrams resulting from quantum many-body effects have been explored plentifully [13, 14, 15, 16, 17, 18, 19, 20]. Most previous discussions assumed that interactions between three and(or) more trapped bosons are negligible so the system is merely controlled by the two-body interaction and tunneling effect which allow bosons to hop around within the optical lattice.

However, it has been an intriguing question of pursuing some exotic phases associated with Hamiltonians with three- or more-body terms [21] for a long time. Quite recently, Büchler *et al.* [22] suggested that polar molecules in optical lattices driven by microwave fields naturally give rise to Hubbard model with strong nearest-neighbor three-body interaction, while the two-body term can be tuned with external fields. This may lead to some interesting quantum phases when generalized to more complicated situations.

In the present work, we discuss the superfluid to Mott-insulator transition of cold bosons in optical lattices with two-and three-body repulsive interactions. We find that in the strong coupling limit, an effective on-site Hamiltonian can be derived with a decoupling mean-field approximation developed in Ref. [16]. We then calculate the energy of this Hamiltonian using perturbation the-

ory and discuss the critical behavior at transition point with Landau order parameter expansion. We find that due to the presence of the three-body interaction, the Mott-insulator areas expand to three-dimensional curved surfaces, and these 3D insulating 'lobes' rotate with respect to a fixed point in the phase space, as more atoms are populated on the lattice sites. We then analyze some experimental parameters corresponding to the theoretical quantities discussed here and suggest some practical ways to verify our results.

II. MEAN-FIELD APPROXIMATION

In this section, we first derive the effective Hamiltonian in the mean-field approximation and then calculate the energy of this Hamiltonian by applying perturbation theory up to the fourth order. The equation of critical curves separating the Mott insulator and superfluid phases are obtained through Landau order parameter expansion for second-order phase transitions.

A. The Effective Hamiltonian

We assume that the atoms are in the lowest band of the optical lattice, thus their behaviors can be described by an (extended) Bose-Hubbard Hamiltonian

$$\hat{H} = -t\sum_{\langle i,j\rangle}\hat{c}_i^\dagger\hat{c}_j + \frac{U}{2}\sum_i\hat{n}_i(\hat{n}_i-1)$$
$$+\frac{W}{6}\sum_i\hat{n}_i(\hat{n}_i-1)(\hat{n}_i-2) - \mu\sum_i\hat{n}_i, \quad (1)$$

where the summation in the first term is done for the nearest neighbors only and $\hat{c}_i^\dagger(\hat{c}_i)$ is the bosonic creation(annihilation) operator with $\hat{n}_i$ the particle number operator for bosons at site i. The parameter t is the hopping term(tunneling amplitude) and $U(W)$ is two(three)-body repulsive interaction strength between bosons. The

*Electronic address: bolun˙chen@mail.bnu.edu.cn
†Corresponding author; Electronic address: spkou@bnu.edu.cn

chemical potential μ is introduced to conserve the number of atoms in the grand-canonical ensemble.

In the *strong coupling limit*, namely, $t \ll \min\{U, W\}$, it is convenient to introduce a superfluid order parameter [16] $\psi = \sqrt{\langle \hat{n}_i \rangle} = \langle \hat{c}_i^\dagger \rangle = \langle \hat{c}_i \rangle$ to construct a consistent mean-field approximation by substituting the hopping term in Eq. (1) as

$$\hat{c}_i^\dagger \hat{c}_j = \langle \hat{c}_i^\dagger \rangle \hat{c}_j + \hat{c}_i^\dagger \langle \hat{c}_j \rangle - \langle \hat{c}_i^\dagger \rangle \langle \hat{c}_j \rangle = \psi(\hat{c}_i^\dagger + \hat{c}_j) - \psi^2. \quad (2)$$

Thus the effective Hamiltonian becomes

$$\begin{aligned}
\hat{H}^{\mathrm{eff}} &= -zt\psi\sum_i(\hat{c}_i^\dagger + \hat{c}_i) + zt\psi^2 N_s + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \\
&\quad + \frac{W}{6}\sum_i \hat{n}_i(\hat{n}_i - 1)(\hat{n}_i - 2) - \mu\sum_i \hat{n}_i, \quad (3)
\end{aligned}$$

where z is the coordination number of optical lattices and N_s is the total number of lattice sites. It can be diagonalized and rewritten with respect to the site index i as

$$\begin{aligned}
\hat{H}_i^{\mathrm{eff}} &= \frac{\overline{U}}{2}\hat{n}_i(\hat{n}_i - 1) + \frac{\overline{W}}{6}\hat{n}_i(\hat{n}_i - 1)(\hat{n}_i - 2) \\
&\quad - \overline{\mu}\hat{n}_i - \psi(\hat{c}_i^\dagger + \hat{c}_i) + \psi^2, \quad (4)
\end{aligned}$$

where dimensionless parameters $\overline{U} = U/zt$, $\overline{W} = W/zt$ and $\overline{\mu} = \mu/zt$ illustrate relative strengths between repulsive interactions (two- and three-body) and tunneling effect (the hopping term t). This on-site Hamiltonian can be applied equally to every lattice site so we will omit the index i in following discussions.

B. Perturbation Theory

In the strong coupling regime, we apply perturbation theory to calculate the energy of Eq. (4). To achieve this, we rewrite Eq. (4) as

$$\hat{H}^{\mathrm{eff}} = \hat{H}^{(0)} + \psi\hat{V} \quad (5)$$

with the unperturbed Hamiltonian $\hat{H}^{(0)} = \frac{\overline{U}}{2}\hat{n}(\hat{n}-1) + \frac{\overline{W}}{6}\hat{n}(\hat{n}-1)(\hat{n}-2) - \overline{\mu}\hat{n} + \psi^2$, and the perturbation $\hat{V} =$

$-(\hat{c}_i^\dagger + \hat{c}_i)$, representing the small kinetic energy of bosons near the insulating phase. The ground-state energy of $\hat{H}^{(0)}$ is

$$\begin{aligned}
E_g^{(0)} &= \left\{ E_n^{(0)}|_{n=0,1,2,\ldots} \right\}_{\min} \\
&= \frac{\overline{U}}{2}g(g-1) + \frac{\overline{W}}{6}g(g-1)(g-2) - \overline{\mu}g, \quad (6)
\end{aligned}$$

where $E_n^{(0)}$ denotes the unperturbed energy of states with integer fillings and g is an integer specifying the average particle number on a lattice site.

In the occupation number basis, the odd powers of the expansion of Eq. (5) with respect to ψ vanish. Therefore, the correction to the energy can be calculated to the second-order

$$E_g^{(2)} = \psi^2 \sum_{n \neq g} \frac{\left| \langle g | \hat{V} | n \rangle \right|^2}{E_g^{(0)} - E_n^{(0)}} = a_2\psi^2 \quad (7)$$

with

$$\begin{aligned}
a_2 &= \left[\frac{g}{(g-1)\overline{U} + \frac{1}{2}(g-1)(g-2)\overline{W} - \overline{\mu}} \right. \\
&\quad \left. + \frac{g+1}{\overline{\mu} - g\overline{U} - \frac{1}{2}g(g-1)\overline{W}} \right], \quad (8)
\end{aligned}$$

and to the fourth-order

$$\begin{aligned}
E_g^{(4)} &= \sum_{n,p,q \neq g} \left| \langle g | \hat{V} | n \rangle \right| \left[-E_g^{(2)} \frac{\left| \langle n | \hat{V} | g \rangle \right|}{\left(E_g^{(0)} - E_n^{(0)} \right)^2} \right. \\
&\quad \left. + \frac{\left| \langle n | \hat{V} | p \rangle \right|}{E_g^{(0)} - E_n^{(0)}} \frac{\left| \langle p | \hat{V} | q \rangle \right|}{E_g^{(0)} - E_p^{(0)}} \frac{\left| \langle q | \hat{V} | g \rangle \right|}{E_g^{(0)} - E_q^{(0)}} \right] \\
&= a_4\psi^4 \quad (9)
\end{aligned}$$

with

$$a_4 = \frac{g(g-1)}{\left[(g-1)\overline{U} + \frac{1}{2}(g-1)(g-2)\overline{W} - \overline{\mu}\right]^2 \left[(2g-3)\overline{U} + (g-2)^2\overline{W} - 2\overline{\mu}\right]}$$
$$+ \frac{(g+1)(g+2)}{\left[\overline{\mu} - g\overline{U} - \frac{1}{2}g(g-1)\overline{W}\right]^2 \left[2\overline{\mu} - (2g+1)\overline{U} - g^2\overline{W}\right]}$$
$$- \left[\frac{g}{(g-1)\overline{U} + \frac{1}{2}(g-1)(g-2)\overline{W} - \overline{\mu}} + \frac{g+1}{\overline{\mu} - g\overline{U} - \frac{1}{2}g(g-1)\overline{W}}\right] \times$$
$$\left[\frac{g}{\left((g-1)\overline{U} + \frac{1}{2}(g-1)(g-2)\overline{W} - \overline{\mu}\right)^2} + \frac{g+1}{\left(\overline{\mu} - g\overline{U} - \frac{1}{2}g(g-1)\overline{W}\right)^2}\right]. \quad (10)$$

Here, $|n\rangle, |p\rangle, |q\rangle$ denote unperturbed states with n, p, q particles.

C. Landau Order Parameter Expansion

We then follow the ordinary procedure for second order phase transitions by writing the ground-state energy $E_g(\psi) = E_g^{(0)} + E_g^{(2)} + E_g^{(4)} + ...$ as an expansion in ψ, with an implication that the superfluidity cannot be large in the strong coupling region:

$$E_g(\psi) = a_0\left(g, \overline{U}, \overline{W}, \overline{\mu}\right) + \left[1 + a_2\left(g, \overline{U}, \overline{W}, \overline{\mu}\right)\right]\psi^2$$
$$+ a_4\left(g, \overline{U}, \overline{W}, \overline{\mu}\right)\psi^4 + \mathcal{O}\left(\psi^6\right). \quad (11)$$

By minimizing Eq. (11) with respect to the superfluid order parameter ψ, we obtain the critical condition $1 + a_2 = 0$ signifying the boundary that separates insulator and superfluid phases, which yields

$$\overline{\mu}_\pm = \frac{1}{2}\left[(2g-1)\overline{U} + (g-1)^2\overline{W} - 1\right] \pm \frac{1}{2}\sqrt{\Delta} \quad (12)$$

with

$$\Delta = \overline{U}^2 + (g-1)^2\overline{W}^2 + 2(g-1)\overline{UW}$$
$$- 2(2g+1)\overline{U} - 2(2g+1)(g-1)\overline{W} + 1, \quad (13)$$

where the subscript $\pm$ denotes the upper and lower halves of the Mott insulating regions in phase space. The parameter Δ will play a significant role in determining phase diagrams, which will be discussed in detail in the next section.

For given particle number g, the weak superfluidity is

$$\psi^2 = -\frac{1 + a_2}{2a_4}, \quad (14)$$

which is illustrated in Fig. 1. Here, we would like to make a remark on our decoupling-Landau expansion scheme. This method was originally introduced[16] as an alternative way of the usual Bogoliubov approximation, which did not predict the phase transition. Instead of considering number fluctuations with respect to the number of condensed atoms in Bogoliubov treatment, decoupling method approximates the kinetic term as site-independent and weak, thus it reveals the expected transition. But it only works well in the *strong-coupling limit* ($U/t, W/t \gg 1$), making hopping as perturbations in expansion of $E(\psi)$. It cannot describe the system properly in the weak-coupling limit, as shown in right plot of Fig. 1: ψ^2 tends to decrease towards zero as repulsions decline. Also, in the case of $g = 1, U = 0$, ψ^2 exhibits strange behavior which is really beyond our approach (the system should be a weak-interaction BEC in this sense, we shall discuss it elsewhere). The incorrectness stems from the limited effective range of our approach.

III. THE PHASE DIAGRAMS

In this section, we present the phase diagrams based on results obtained in the previous section and demonstrate their physical meanings with the help of Eq. (13).

According to Eq. (12), physically acceptable solutions of the reduced chemical potential $\overline{\mu}$ require that $\Delta \geq 0$. This restriction, which guarantees $\overline{\mu}$ being real-valued and the existence of Mott insulating phases, can be visualized in Fig. 2 as we set Eq. (13) to be zero. In fact, solutions to $\Delta = 0$ are a set of parallel lines in the $\overline{U}$-$\overline{W}$ plane. They divide the plane into two parts: areas to their right correspond to $\Delta > 0$, which implies the appearance of the Mott-insulating phase; areas to their left correspond to $\Delta < 0$, which implies the appearance of the superfluid phase. Areas with negative values of ($\overline{U}$ or $\overline{W}$) are not shown since we only consider repulsive interactions among atoms.

The critical line is perpendicular to the $\overline{U}$-axis with an intercept of $\overline{U}_C = 5.83$ when $g = 1$, which is exactly the transition point of system with pure two-body interaction. It seems to be contradictory, since according to Eq. (1), both the two-body and the three-body terms have to vanish at $g = 1$, and the system ought to behave as a non-interacting BEC. We can understand it in the following way:

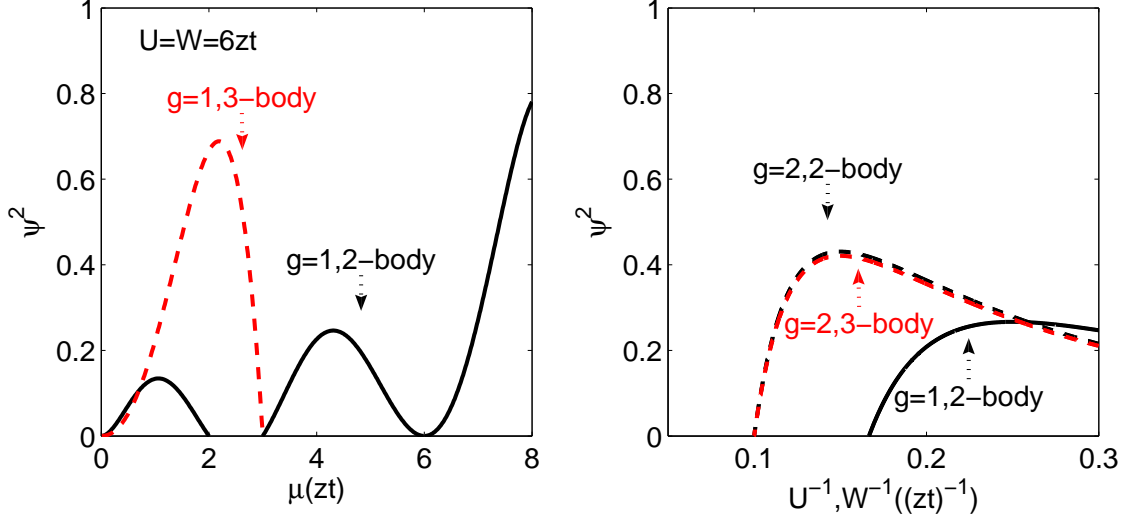Although the on-site repulsion $U\hat{n}_i(\hat{n}_i - 1)$ vanishes at

FIG. 1: (Color online) Illustrations of superfluid order parameters ψ^2 according to Eq. (14). Left: with fixed repulsion and varying chemical potential $\overline{\mu}$ at $g = 1$. The black line denotes $\overline{U} = 6, \overline{W} = 0$; The red dash line denotes $\overline{U} = 0, \overline{W} = 6$. Right: with $\overline{\mu} = (g - \frac{1}{2})\overline{U} + \frac{1}{2}(g-1)^2\overline{W}$ and varying $\overline{U}^{-1}, \overline{W}^{-1}$. The solid line denotes $g = 1$, the dash lines denote $g = 2$.
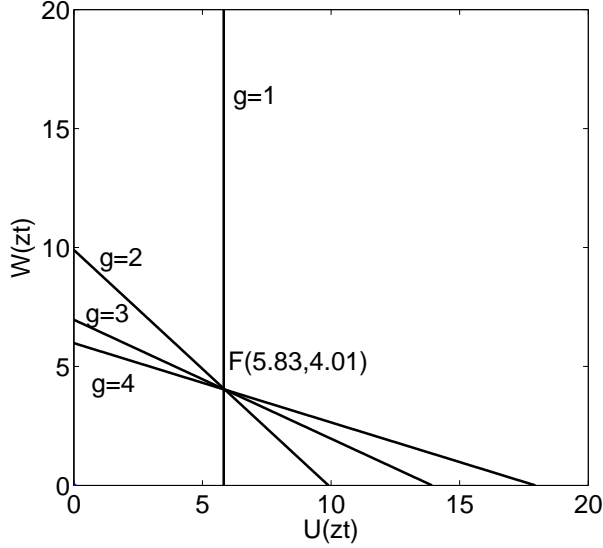

FIG. 2: Illustration of solutions to $\Delta = 0$ with different occupancy g. The critical lines are tilting down as g increases and all of them intersect around a fixed point point $F(5.83, 4.01)$.

single occupancy, two-body interactions can take place due to weak (perturbative) tunneling effect. It enables one boson to 'jump' from one site to its nearest neighbors, so the on-site repulsion between two bosons appears again, raising energy and may forbid the occupation of an additional atom if U is strong enough. In short, when hoppings are added as perturbations (the Landau expansions in ψ^2), the condensate can exhibit a weak superfluid phase. In the large U/t regime, hoppings are prohibited

and the condensate becomes insulating.

Similarly, three-body interactions $W\hat{n}_i(\hat{n}_i - 1)(\hat{n}_i - 2)$ may appear as two (or more) bosons successively move onto an occupied site. But these processes are hidden in higher-order terms (ψ^4 and above) in our kinetic-perturbation expansion, thus can be neglected here. This explains the absence of three-body interactions at $g = 1$. Hence, the condensate can be described as a weak-interacting BEC with finite two-body repulsions and can have the Mott transition.

When $g = 2$, the U-term is recovered while the W-term can emerge by adding hopping perturbations (with one atom jumping). So the system can either be a weak superfluid or an insulator, depending on the ratio U/t and W/t.

In addition, three-body term will surpass the two-body one gradually as g increases. From Fig. 2, we can see that as there are more particles on sites, intercepts of the critical lines to $\overline{W}$-axis become smaller; when $g \to \infty$, the intercept goes to $\overline{W}_C = 4.01$. In fact, all the lines with different g intersect around the point $F(5.83, 4.01)$ and rotate with respect to it: from being perpendicular to the $\overline{U}$-axis when $g = 1$ to being parallel to the $\overline{U}$-axis when $g \to \infty$.

This behavior can be straightforwardly explained from the dispersion relation (obtained in a similar way as in

Ref. [16] by using an effective action method)

$$\hbar\omega_\pm = \frac{1}{2}\left[(2g-1)U + (g-1)^2 W - \epsilon_{\boldsymbol{k}} - 2\mu\right] \pm$$
$$\frac{1}{2}\left[U^2 + (g-1)^2 W^2 + 2(g-1)UW - \right.$$
$$\left. 2(2g+1)\epsilon_{\boldsymbol{k}}U - 2(2g+1)(g-1)\epsilon_{\boldsymbol{k}}W + \epsilon_{\boldsymbol{k}}^2\right]^{1/2},$$
$$(15)$$

where $\epsilon_{\boldsymbol{k}} = 2t\sum_{i=1}^{d}\cos(k_i a)$, "$\pm$" denote excitations of quasi-particles (adding particles to sites) and quasi-holes (removing particles from sites), respectively. Furthermore, by subtracting the two solutions, we can obtain the energy gap

$$\Delta_{\boldsymbol{k}}^2 = U^2 + (g-1)^2 W^2 + 2(g-1)UW -$$
$$2(2g+1)\epsilon_{\boldsymbol{k}}U - 2(2g+1)(g-1)\epsilon_{\boldsymbol{k}}W + \epsilon_{\boldsymbol{k}}^2.$$
$$(16)$$

At the transition point, $\Delta_{\boldsymbol{k}}^2 = 0$ and we have

$$W_C = \frac{-U_C + \left[2g + 2\sqrt{g(g+1)} + 1\right]\epsilon_{\boldsymbol{k}}}{g-1}. \qquad (17)$$

This equation shows the g-dependence U_C and W_C: as g grows, the slope $(g-1)^{-1}$ decreases; so that U_C increases while W_C declining to a fixed value at about $4\epsilon_{\boldsymbol{k}}$. For $\boldsymbol{k} = 0$, $\epsilon_{\boldsymbol{k}} = zt$, the dispersion relation(15) becomes the phase boundary equation(12), while $\Delta_{\boldsymbol{k}}^2$ turning to $z^2 t^2 \Delta$. Let $\Delta = 0$, the relation between $\overline{U}_C$ and $\overline{W}_C$ is

$$\overline{U}_C + (g-1)\overline{W}_C = 2g + 1 + 2\sqrt{g(g+1)}. \qquad (18)$$

When $g \to \infty$ and $\overline{U}_C = 0$, $\overline{W}_C \approx 4$; when $g = 1$, $\overline{W}_C$ is divergent and $\overline{U}_C \approx 5.83$.

The physical meanings of this rotation of critical lines may be easier to comprehend when we plot the complete phase diagrams in three-dimensions in Fig. 3. The well known Mott insulating 'lobes' now expand to a set of curved surfaces, meanwhile the transition points become the critical lines in Fig. 2. As g increases, these surfaces rotate with respect to the fixed point $F(5.83, 4.01)$.

Figure 4 shows the superfluid phase and Mott insulator lobes of condensate with pure two-body and three-body interactions, respectively. As we can see, the three-body interaction enlarges the areas of Mott lobes significantly, which is contrary to pure two-body situation, whose lobes shrink as g increases: According to Eq. (12) and (13), breadths of different U-lobes are 1 while W-lobes' breadths are expanding as $(g-1)$ in the unit of μ/U and μ/W, respectively.

IV. THE EXPERIMENTAL PARAMETERS AND SUGGESTIONS

The trapping potential is the sum of a homogeneous periodic lattice potential formed by three orthogonal, independent standing laser fields with a tunable barrier
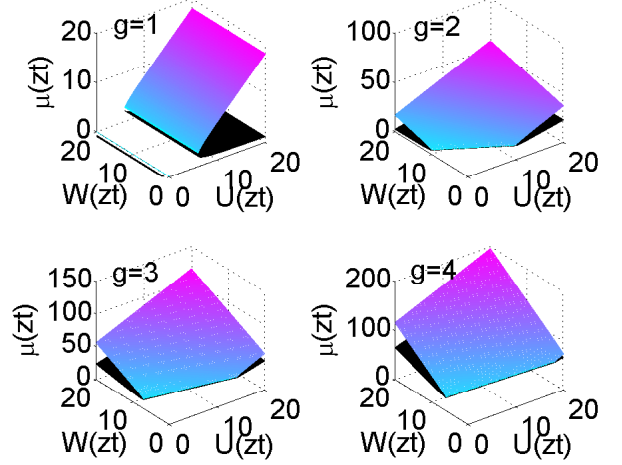

FIG. 3: (Color online) Mott-insulating 'lobes' in 3D phase space. The areas enclosed within lobes indicate insulating phase. Space outside these curved surfaces is superfluid phase.
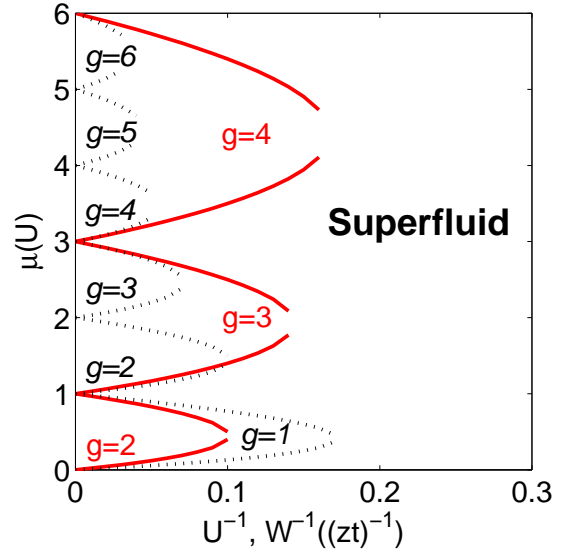

FIG. 4: (Color online) Phase diagrams of superfluid-Mott insulator transition with pure two-and three-body interactions. The red lines are associated with pure three-body interaction and the black dot lines are associated with pure two-body interaction.

height V_0 [20]. For a deep optical lattice this sine-like trap can be approximated as a harmonic well as

$$V(x,y,z) = V_0\left(\sin^2 kx + \sin^2 ky + \sin^2 kz\right)$$
$$\approx V_0 k^2\left(x^2 + y^2 + z^2\right), \qquad (19)$$

where $k = 2\pi/\lambda$ is the wave vector with λ the wave length of the laser. The Wannier function at the lowest band in

the well can be approximated as a Gaussian ground-state

$$w(\boldsymbol{r}) = \left(\frac{\alpha^2}{\pi}\right)^{\frac{3}{4}} e^{-\frac{1}{2}\alpha^2 \boldsymbol{r}^2}, \qquad (20)$$

where $\alpha^{-1} = \left(2mV_0 k^2/\hbar^2\right)^{-\frac{1}{4}}$ is the characteristic length of harmonic oscillators. The interaction parameter U and W are thus given by integrals over the Wannier function [17]

$$U = g_2 \int \mathrm{d}\boldsymbol{r} \, |w(\boldsymbol{r})|^4 = \sqrt{\frac{8}{\pi}} k a_s E_r \left(\frac{V_0}{E_r}\right)^{\frac{3}{4}}, \qquad (21)$$

and

$$\begin{aligned} W &= g_3 \int \mathrm{d}\boldsymbol{r} \, |w(\boldsymbol{r})|^6 = g_3 \left(\frac{V_0}{E_r}\right)^{\frac{3}{2}} \left(\frac{k^2}{\sqrt{3}\pi}\right)^3 \\ &= \left(\sqrt{3}\pi\right)^{-3} \ln\left(C\eta^2\right) \frac{ma_s^2}{\hbar^2} U^2, \end{aligned} \qquad (22)$$

where $g_2 = 4\pi\hbar^2 a_s/m$ is the coupling constant of the delta-type repulsion between two bosons with a_s the s-wave scattering length and m the mass of bosons, while $E_r = \hbar^2 k^2/2m$ is the recoil energy. The three body coupling constant has been calculated in a previous work [23] as

$$g_3 = \frac{16\pi\hbar^2}{m} a_s^4 \ln\left(C\eta^2\right), \qquad (23)$$

where $\eta = \sqrt{|\psi|^2 a_s^3}$ is the dilute gas parameter and the constant C in the argument of the logarithm can be determined by applying a microscopic description demonstrated in [21]. In the limit $V_0 \gg E_r$, the tunneling amplitude t can be obtained from the exact result for the width of the lowest band in the one-dimensional Mathieu equation as [17]

$$t = \frac{2}{\sqrt{\pi}} E_r \left(\frac{V_0}{E_r}\right)^{\frac{3}{4}} e^{-2\sqrt{\frac{V_0}{E_r}}}. \qquad (24)$$

Combining Eq. (21), (22) and (24), we obtain the relation between dimensionless interaction strengths $\overline{W}$ and $\overline{U}$ as

$$\overline{W} = (3\pi)^{-\frac{3}{2}} \ln\left(C\eta^2\right) \left(\frac{V_0}{E_r}\right)^{\frac{3}{4}} e^{-2\sqrt{\frac{V_0}{E_r}}} a_s^2 k^2 \overline{U}^2, \qquad (25)$$

where $a_s^2 k^2$ ranges from 10^{-8} to 10^{-2} in current experiments [24]. As we can see, in this context, the strength of three-body interaction is much weaker than its two-body counterpart, which means that three-body effects can hardly be observed. This is consistent with the current experiments where the manipulation of two-body interactions $\overline{U}$ is accomplished through changing the depth of the optical well V_0.

However, as Ref. [22] pointed out, by loading the polar molecules into the optical lattice and adding an external microwave field, one can achieve a situation where only observable three-body interaction exists. It may open a promising route for an experimental study of controlling different interatomic repulsions individually, and the system can be possibly prepared with pure three-body interaction. Moreover the experimental techniques like Feshbach resonance for molecules [25] and the rapid progress in dipolar condensate [26] provide us more opportunities to tackle the many-body problems in cold atomic gases. In that case, the above discussions on the exotic quantum phases and the new type of Mott-Hubbard transition can be examined.

V. CONCLUSIONS

In this paper, the superfluid-insulator transition with many-body interactions between optically-trapped ultracold bosonic atoms is discussed. We find the extension of the Mott-insulating areas and the existence of a fixed point in phase space. Finally, we explore the possibility of realizing the theoretical predictions and suggest some experimental means to test our results.

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